Pores for thought: generative adversarial networks for stochastic reconstruction of 3D multi-phase electrode microstructures with periodic boundaries

 Authors: Andrea Gayon-Lombardo, L. Mosser, N. Brandon, S. J. Cooper

Abstract

The generation of multiphase porous electrode microstructures is a critical step in the optimisation of electrochemical energy storage devices. This work implements a deep convolutional generative adversarial network (DC-GAN) for generating realistic n-phase microstructural data. The same network architecture is successfully applied to two very different three-phase microstructures: A lithium-ion battery cathode and a solid oxide fuel cell anode. A comparison between the real and synthetic data is performed in terms of the morphological properties (volume fraction, specific surface area, triple-phase boundary) and transport properties (relative diffusivity), as well as the two-point correlation function. The results show excellent agreement between datasets and they are also visually indistinguishable. By modifying the input to the generator, we show that it is possible to generate microstructure with periodic boundaries in all three directions. This has the potential to significantly reduce the simulated volume required to be considered “representative” and therefore massively reduce the computational cost of the electrochemical simulations necessary to predict the performance of a particular microstructure during optimisation.